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FILE COVERS 1907 - 21 Jul 2010 VOL 153 ISS 4 FILE LAST UPDATED: 20 Jul 2010 (20100720/ED) REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2010 USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2010

CAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2010.

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## http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que 125 L3 STR



NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

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L15 STR

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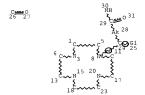


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L40 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2010 ACS on STN ACCESSION NUMBER: 2008:1282714 CAPLUS Full-text

DOCUMENT NUMBER: 149:507859

TITLE: Peptide conjugates with signal entities for diagnosing

apoptosis

INVENTOR(S): Port, Marc; Rousseaux, Olivier; Muller, Robert; Burtea, Carmen

PATENT ASSIGNEE(S): Guerbet, Fr.

SOURCE: PCT Int. Appl., 73pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: French FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

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                       A1 20100610
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                                                                20090928
PRIORITY APPLN. INFO.:
                                          FR 2007-54086
                                                            A 20070328
                                          WO 2008-EP53447
                                                            W 20080321
```

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT MARPAT 149:507859 OTHER SOURCE(S):

- AB The invention discloses compds. Signal-Link-Peptide [Signal = signal entity; Link = absent, linker; Peptide = peptide comprising an apoptosis-targeting peptide, the apoptosis-targeting peptide being selected from X1-X2-X3-X4-X5-X6 (X1, X2 = leucine, isoleucine; X3, X4 = lysine; X5 = proline; X6 = phenylalanine), advantageously LIKKPF, and functional equivalent thereof; D-A-H-S-X7-S (X7 = phenylalanine, leucine); P-G-D-L-X8-X9 (X8 = serine, valine; X9 = threonine, arginine); H-G-X10-L-S-X11 (X10 = aspartic acid, histidine; X11 = threonine, isoleucine); VLGERG], and the pharmaceutically acceptable salts thereof. Compound preparation is included.
- IΤ 1064074-04-9
  - RL: RCT (Reactant); RACT (Reactant or reagent) (peptide conjugates with signal entities for diagnosing apoptosis)
- RN 1064074-04-9 CAPLUS
- Gadolinate(3-), [N-[4-(carboxy-κ0)-4-[4,7,10-tris[(carboxy-CN
  - κO)methyl]-1,4,7,10-tetraazacyclododec-1-vl-
  - $\kappa$ N1,  $\kappa$ N4,  $\kappa$ N7,  $\kappa$ N10]-1-oxobutyl]-L- $\alpha$ -aspartyl-L-
  - alanyl-L-histidyl-L-servl-L-phenylalanyl-L-serinato(6-)|-, hydrogen (1:2)

PAGE 1-A

●2 H+

PAGE 1-B

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L40 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2010 ACS on STN ACCESSION NUMBER: 2008:1191058 CAPLUS Full-text

DOCUMENT NUMBER:

149:420505

TITLE: Peptide ligands for phosphatidylserine for use in the

diagnostic imaging of apoptosis

INVENTOR(S): Port, Marc; Rousseaux, Olivier; Muller, Robert;

Burtea, Carmen Guerbet, Fr.

SOURCE: Fr. Demande, 63pp. CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT ASSIGNEE(S):

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PRIORITY APPLN. INFO.:
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                                                              A 20070328
                                          WO 2008-EP53447
                                                             W 20080321
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ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

Synthetic peptides that can bind phosphatidylserines and that can be used in the imaging of areas of apoptosis in disease diagnosis are described. These peptides are conjugated with a chelating agent for the delivery of detectable metal ion. The peptide has the general formula: X1X2KKPF (X1, X2 = independently isoleucine or leucine) and may be coupled with a signal peptide. Functional equivalent include: DAHSX7S (X7 = phenylalanine or leucine), PGDLX8X9 (X8 = serine or valine, X9=threonine or arginine), and HGX10LSX11 (X10 = aspartic acid or histidine, X11 = threonine or isoleucine), and VLGERG.

1064074-04-9DP, peptide conjugates RL: ARG (Analytical reagent use); DGN (Diagnostic use); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP

(peptide ligands for phosphatidylserine for use in diagnostic imaging of apoptosis)

RN 1064074-04-9 CAPLUS

(Preparation); USES (Uses)

CN Gadolinate(3-),  $[N-[4-(carboxy-\kappa 0)-4-[4,7,10-tris](carboxy$ κO)methvll-1,4,7,10-tetraazacvclododec-1-vl-

 $\kappa N1, \kappa N4, \kappa N7, \kappa N10] - 1 - 0 \times 0 \times 0 \times 1 - L - \alpha - \alpha \times 0 \times 1 - L - \alpha$ 

alanyl-L-histidyl-L-seryl-L-phenylalanyl-L-serinato(6-)]-, hydrogen (1:2) (CA INDEX NAME)

PAGE 1-A

●2 H+

PAGE 1-B

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L40 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2010 ACS on STN ACCESSION NUMBER: 2004:1156521 CAPLUS Full-text

DOCUMENT NUMBER: 142:94136 TITLE:

Preparation of peptidyl gadolinium contrast agents having specific high-relaxivity

Port, Marc: Rousseaux, Olivier: Corot, Claire; INVENTOR(S):

Prigent, Philippe; Lancelot, Eric PATENT ASSIGNEE(S): Guerbet, Fr.

SOURCE:

PCT Int. Appl., 179 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

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PRIORITY APPLN. INFO.:
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ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT The invention relates to novel compds, and pharmaceutical compns, that are useful for the diagnosis of many pathologies, in particular cardiovascular, cancer-related and inflammatory pathologies. These compds. comprise a component for targeting a pathol. region linked to a detection component which is effective in diagnostic terms. The detection component is typically an MRI contrast agent, an X-ray contrast agent, or an entity containing a radioisotope or able to be detected by ultrasound or by optical imaging. Compds. Bx-Lz-(HR Ch)y (B is a biovector, L is a linker, HR Ch is a chelate, and x, y, z are 1-8), and their salts with pharmaceutically-acceptable acids or bases, are claimed. Thus, a gadolinium-complexed 1,4,7,10tetraazacyclododecane derivative was prepared and coupled with peptide H-Pro-Leu-Gly-NHOH. A bis-folate derivative shows very good molar relaxivity (53 mM-1.s-1 at 60 MHz).

596121-51-6P 596121-92-5P

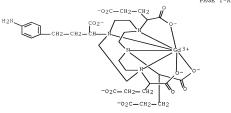
RL: DGN (Diagnostic use); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of peptidyl gadolinium contrast agents having specific high-relaxivity)

596121-51-6 CAPLUS RN

CN Gadolinate(4-),  $[\alpha-[2-(4-aminophenyl)ethyl]$ α', α'', α'''-tris(2-carboxvethvl)-1,4,7,10tetraazacyclododecane-1, 4, 7, 10-tetraacetato(7-)-KN1, KN4, KN7, KN10, KO4, KO7, KO101-, tetrasodium (9CI) (CA INDEX NAME)





PAGE 2-A

●4 Na+

RN 596121-92-5 CAPLUS

PAGE 1-A

PAGE 1-B

PAGE 1-C

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PAGE 2-A

PAGE 2-B

IT 596121-78-7P 596121-90-3P 596121-94-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation of peptidyl gadolinium contrast agents having specific high-relaxivity)

RN 596121-78-7 CAPLUS

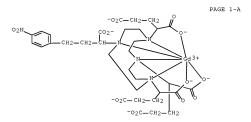
CN Gadolinate(4-),  $[\alpha, \alpha', \alpha''-tris(2-carboxyethyl)-$ 

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1,4,7,10-tetraacetato(7-)-

κN1, κN4, κN7, κN10, κO1, κO4, κO7]-,

tetrahydrogen (9CI) (CA INDEX NAME)



PAGE 2-A

●4 H+

PAGE 1-C

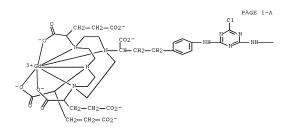
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PAGE 2-B

RN 596121-94-7 CAPLUS

CN Gadolinate(8-), [ $\mu$ -[[ $\alpha$ , $\alpha$ ''''-[(6-chloro-1,3,5-triazine-2,4-

diyl)bis(imino-4,1-phenylene-2,1ethanediyl)|bis(a',a'',a'''-tris(2-carboxyethyl)-1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraacetatokNl,kNl,kNl,kNl,kNl,kOd,kOd,kOl,kOll)| (14-)||di-, octahydrogen (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L40 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2010 ACS on STN ACCESSION NUMBER: 2003:719481 CAPLUS Full-text DOCUMENT NUMBER: 139:254313

TITLE: Gadolinium chelate oligomers, their use as contrast products in magnetic resonance imaging and their

synthetic intermediates

INVENTOR(S): Nachman, Isabelle; Port, Marc; Raynal, Isabelle;

Rousseaux, Olivier

PATENT ASSIGNEE(S): Guerbet SA, Fr. PCT Int. Appl., 122 pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE: Patent. LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

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ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT GI

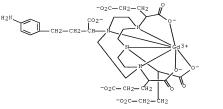
- \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT \*
- AB The invention concerns macrocyclic high-relaxivity gadolinium chelate oligomers of formula W-(A)m, wherein W, A and m represent a wide variety of polynuclear gadolinium DOTA amide analogs, and their use as contrast products with vascular remanence for magnetic resonance imaging. Example compds., e.g., I, are prepared and exhibit strong relaxivity.
- 596121-51-6P 596121-52-7P 596121-53-8P 596121-78-7P 596121-86-7P 596121-88-9P 596121-90-3P 596121-93-6P 596121-94-7P 596122-02-0P
  - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of gadolinium chelate oligomers as contrast agents in magnetic resonance imaging)

- RN 596121-51-6 CAPLUS
- Gadolinate (4-),  $[\alpha-[2-(4-aminophenvl)]$  ethvl]- $\alpha', \alpha'', \alpha'''$ -tris(2-carboxyethyl)-1,4,7,10-

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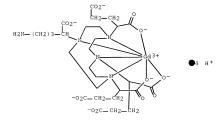


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●4 Na+

RN 596121-52-7 CAPLUS

CN Gadolinate(4-), [α-(3-aminopropyl)-α',α'',α'''tris(2-carboxyethyl)-1,4,7,10-tetraazacyclododecane-1,4,7,10tetraacetato(7-)-κN1,κN1,κN10,κΟ4, kappa
.07,κ010]-, tetrahydrogen (9C1) (CA INDEX NAME)



- - 4,1-butanediyl]imino(1-oxo-2,1-ethanediyl)imino(2,4,6-tribromo-5,1,3-benzenetriyl)bis[carbonyl1(2,3-dihydroxypropyl)imino]]]]hexakis[1-deoxyhexitolato][3-]]- [9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

PAGE 1-C

PAGE 2-A

RN 596121-78-7 CAPLUS

CN Gadolinate(4-), [ $\alpha$ ,  $\alpha$ ',  $\alpha$ ''-tris(2-carboxyethy1)-

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O2C-CH2-CH2

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O2C-CH2-CH2

O2C-CH2-CH2

O2C-CH2-CH2

PAGE 2-A

●4 H+

RN 596121-86-7 CAPLUS

CN

Gadolinium, [[1,1",1"',1"',1"''-[13-[3-[(1,1-dimethylethoxy)carbonyl]amino]propyl]-3,6,9,15-tetraazabicyclo[9.3.1]pentadeca-1(15),11,13-triene-3,6,9-triyl-N3, KN6, KN9, KN15[tris[[4-(carboxy-KO)-1-oxo-4,1-butanediyl]mino[1-oxo-2,1-ethanediyl]mino[2,4,6-tribromo-5,1,3-benzenetriyl]bis[carbonyl[(2,3-dihydroxypropyl)]mino[]]]hexakis[1-deoxyhexitolato][(3,3-]-[9(C]) (CA INDEX NAME)

PAGE 1-A

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PAGE 2-A

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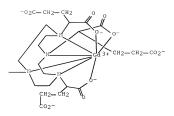
PAGE 2-B

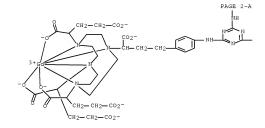
RN 596121-88-9 CAPLUS

CN Gadolinate(12-), [µ3-[[α,α''',α''''-[1,3,5-triazine-2,4,6-triyltris(imino-4,1-phenylene-2,1-ethanediyl)]tris[α',α'',α'''-tris(2-carboxyethyl)-1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraacetato-KNl, KN3, KN7, KN10, KO7, KO10](
21-)]tri-, dodecahydrogen (9CI) (CA INDEX NAME)

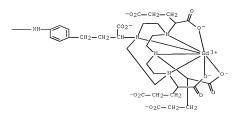
PAGE 1-A

PAGE 1-B





PAGE 2-B



PAGE 3-A ●12 H+

596121-90-3 CAPLUS

RN

Gadolinium, [[1,1',1'',1''',1'''',1'''',1''''',1''''',1''''',1''''',1''''' CN '''',1''''''-[[13-[3-[[(1,1dimethylethoxy)carbonyl]amino]propyl]-3,6,9,15tetraazabicyclo[9.3.1]pentadeca-1(15),11,13-triene-3,6,9-triylκN3, κN6, κN9, κN15] tris[[4-(carboxy-κ0)-1-oxo-4,1-butanediyl]imino(1-oxo-2,1-ethanediyl)imino(2,4,6-tribromo-5,1,3benzenetriyl)bis(carbonylnitrilo)]]dodecakis[1-deoxyhexitolato]](3-)]-(9CI) (CA INDEX NAME)

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PAGE 2-B

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CRN 76-05-1 CMF C2 H F3 02

RN 596121-94-7 CAPLUS
CN Gadolinate(8-),  $[\mu-[[\alpha,\alpha''''-[(6-\text{chloro-1},3,5-\text{triazine-2},4-\text{diyl})]\text{bis}(\min-0,1-\text{phenylene-2},1-\text{ethanediyl})]\text{bis}[\alpha'',\alpha''',\alpha'''-\text{tris}(2-\text{carboxyethyl})-1,4,7,10-\text{tetraazacyclododecane-1},4,7,10-\text{tetraacetato-kNl},kMl,kN7,kNl0,kO4,kO7,kO10]]($ 

14-)]]di-, octahydrogen (9CI) (CA INDEX NAME)

PAGE 1-A

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CO2
NH

NH

NH

NH

NH

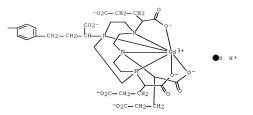
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NH

NH

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CH2-CH2-CO2
CH2-CH2-CO2-

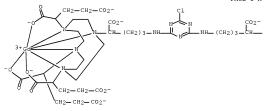
PAGE 1-B



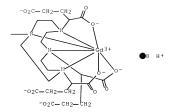
RN 596122-02-0 CAPLUS

CN Gadolinate(8-), [µ-[[a,a''''-[(6-chloro-1,3,5-triazine-2,4-diyl)bis(imino-3,1-propanediyl)]bis[a',a'',a'''-tria(2-carboxyethyl)-1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraacetato-KN1,KN4,KN7,KN10,KO4,KO7,KO10]](
14-)]ldi-, octahydrogen (9CI) (CA INDEX NAME)

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PAGE 1-B



OS.CITING REF COUNT: THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD

(9 CITINGS)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L40 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2003:718469 CAPLUS Full-text DOCUMENT NUMBER: 140:205744

TITLE: Thermodynamic and structural properties of Eu3+, Gd3+

and Tb3+ complexes with

1, 4, 7, 10-tetra(2-glutarvl)-1, 4, 7, 10tetraazacyclododecane in solution: EXAFS,

luminescence, potentiometric studies, and quantum

calculations

Moreau, Juliette; Guillon, Emmanuel; Aplincourt, AUTHOR(S):

Philippe; Pierrard, Jean-Claude; Rimbault, Jean; Port,

Marc; Aplincourt, Michel

GRECI, Universite de Reims Champagne-Ardenne, Reims, CORPORATE SOURCE:

51687/2, Fr.

European Journal of Inorganic Chemistry (2003), (16), SOURCE: 3007-3020

CODEN: EJICFO: ISSN: 1434-1948

Wiley-VCH Verlag GmbH & Co. KGaA

Journal DOCUMENT TYPE:

LANGUAGE: English AB

PUBLISHER:

The stability of the various complexes formed by racemic solns. of the title ligand (L) with Gd3+, Eu3+ and Tb3+ was investigated by potentiometry. The reaction of complexation proceeds through the quick formation of metastable species leading, after a slow reorganization of the macrocycle, to thermodynamically stable complexes. The mean nos. of water mols. coordinated to the lanthanides were determined by luminescence and EXAFS spectroscopy. This last method, applied to solns. of complexes, allowed to precisely determine the nature of the atoms that surround the metal atom and the distance between the lanthanide ion and the various ligands. These structural data that are in good agreement with the results found using quantum mechanics allow to propose a reaction mechanism, from the hydrated lanthanide ion to the final stable complexes through intermediate species. The specific stability of these final complexes arises from the formation of transitory bonds between the metal ion and two pendant arms, which bear carboxylate groups. The stability consts. of the final complexes have high values [log  $\beta$ 110(EuL5-) = 24.01; log  $\beta$ 110(GdL5-) = 24.03; log  $\beta$ 110(TbL5-) = 23.97]. This induces a

notable in vivo dissociation inertness, which is essential for a potential contrast agent in magnetic resonance imaging.

660831-55-0 660831-56-1

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(europium(3+), gadolinium(3+) or terbium(3+) complexation with tetra(glutaryl)-tetraazacyclododecane in aqueous solution from EXAFS, luminescence, potentiometry and quantum calcns.)

660831-55-0 CAPLUS RN

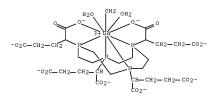
Gadolinate(5-), pentaagua(y,y',y'',y'''-CN tetracarboxy-1,4,7,10-tetraazacyclododecane-1,4,7,10-tetrabutanoato(8-)κN1, κN4, κN7, κN10]-, hexahydrogen (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 660831-56-1 CAPLUS

CN Gadolinate(5-), triaqua(γ,γ''-di(carboxy-κ0)-\( \gamma'', \gamma''' - \text{dicarboxy} - 1, 4, 7, 10 - \text{tetraazacyclododecane} - 1, 4, 7, 10 \( \text{tetraazacyclododecane} - 1, 4, 7, 10 \)

tetrabutanoato(8-)- $\kappa$ N1,  $\kappa$ N4,  $\kappa$ N7,  $\kappa$ N101-. tetrahydrogen (9CI) (CA INDEX NAME)



4 H+

OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD

(6 CITINGS)

REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD, ALL CITATIONS AVAILABLE IN THE RE FORMAT

L40 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2010 ACS on STN

DOCUMENT NUMBER: 134:36356

ACCESSION NUMBER:

2000:881151 CAPLUS Full-text TITLE: Preparation of bicyclic polyamino carboxylic acid and

amide metal complexes for use in medical imaging INVENTOR(S):

Port, Marc PATENT ASSIGNEE(S): Guerbet SA, Fr.

SOURCE: PCT Int. Appl., 38 pp.

CODEN: PIXXD2 DOCUMENT TYPE: Patent

LANGUAGE: French FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

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ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT OTHER SOURCE(S): MARPAT 134:36356
GI

The invention concerns metal chelates of bicyclic macrocycle 3,6,9,15-AB tetraazabicyclo[9.3.1]pentadeca-1(15),11,13-triene acid amide derivs. I [R = -Z-(C6H4Z')p-(C6H4Z')g-C6R1R2R3R4R5; Z = bond, CH2, CH2CONH, (CH2)2NHCO; Z' = bond, O, S, NQ, CH2, CO, CONQ, NQCO, NQCONQ, CONQCH2CONQ; Z'' = bond, CONQ, NQCO, CONQCH2CONQ; p, q = 0-3; R1-R5 are independently H, Br, Cl, iodo, etc.; Q = H , C1-4 alkyl which may be mono- or polyhydroxylated]. Compds. I are useful as medical imaging agents (NMR, scintigraphy, x-ray). More specifically, gadolinium complexes of I are useful as NMR contrast agents. Metal chelates of macrocycle II and its salts are also claimed, including the gadolinium complex. A claimed process for the preparation of I involves reaction of 3,6,9,15-tetraazabicyclo[9.3.1]pentadeca-1(15),11,13-triene with R'02CCHX(CH2)2C02R' (X = leaving group, R' = H, C1-3 alkyl) and hydrolysis of the ester functions when R' # H, followed by reaction with a metal salt or oxide to form the chelate, then reacting the chelate with an amine RNH2 in the presence of an agent to activate the carboxylic acid groups. E.g., a gadolinium(III) complex of 3,6,9,15-tetraazabicyclo[9.3.1]pentadeca-1(15), 11, 13-triene-3,6,9- tri $(\alpha$ -glutaric acid) was prepared by this method.

1(15),11,13-triene-3,6,9-tri $(a-glutaric\ acid)$  was prepared by this method. 1T 311772-48-2P 311772-49-3P 311772-50-6P 311772-52-8P 312280-67-2P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of metal chelates of tetraazabicyclopentadecatriene polyaminocarboxylates and amides as medical imaging agents) 311772-48-2 CAPLUS

kN3, kN6, kN9, kN15) tris[[4-(carboxy-k0)-1-oxo-

RN

CN

4,1-butanediyl]imino(1-oxo-2,1-ethanediyl)imino(2,4,6-tribromo-5,1,3-benzenetriyl)bis(carbonylnitrilo)]]dodecakis[1-deoxyhexitolato]](3-)]-(9CI) (CA INDEX NAME)

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RN 311772-49-3 CAPLUS

CN Gadolinium, [[1,1',1'',1''',1''',1'''-[(3,6,9,15-tetraazahicyclo[9,3.1]pentadeca-[(15),11,3-triene-3,6,9-triylx83,x86,x89,x815)tris[[4-(carboxy-x0)-1-oxo4,1-butanediyl]imino(1-oxo-2,1-ethanediyl)imino(2,4,6-tribromo-5,1,3benzenetriyl)bis[carbonyl[(2,3-dihydroxypropyl)imino]]]hexakis[1-deoxy-Dcalactitolatol][3-)]- [92] (CA INDEX NAME)

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RN 311772-50-6 CAPLUS

4,1-butanediyl]iminomethylene-4,1-phenylenecarbonylimino(2,4,6-tribromo-5,1,3-benzenetriyl)bis[carbonyl[(2,3-dihydroxypropyl)]imino[]]]hexakis[1-dexy-D-galactitolato][(3-)] (9CI) (CA INDEX NAME)

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10/560,830

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RN 311772-52-8 CAPLUS
CO Gadolinium, [[1,1',1'',1''',1''',1'''-[(3,6,9,15tetraazabicyclo[9,3,1]pentadeca-1(15),11,13-triene-3,6,9-triylkN3,kN6,kN9,kN15)tris[[4-(carboxy-k0)-1-oxo4,1-butanediyl]iminomethylene-4,1-phenylenecarbonylimino-4,1phenylenecarbonylimino[2,4,6-tribromo-5,1,3-benzenetriyl]bis[carbonyl[(2,3dihydroxypropyl)imino]]]hexakis[1-deoxy-D-galactitolato]](3-)]- (9CI)
(CA INDEX NAME)

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RN 312280-07-2 CAPLUS

10/560,830

PAGE 1-B

$$\begin{array}{c} \text{CH2-}\\ \text{OH} \\ \text{-CH2-}\\ \text{CH2-}\\ \text{CH2$$

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PAGE 2-B

OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD

(8 CITINGS)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L40 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2010 ACS on STN ACCESSION NUMBER: 1999:392995 CAPLUS Full-text

DOCUMENT NUMBER: 131:67209

TITLE: Metal chelates of macrocyclic polyaminocarboxylic derivatives and their use for diagnostic imaging

PATENT ASSIGNEE(S): Guerbet SA, Fr.
SOURCE: Eur. Pat. Appl., 36 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.						KIND DATE			API	PLICA	DATE					
EP 922700					A1	-	1999	0616	EP	1998		19981209				
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PRIORITY APPLN. INFO.:			FR	1997-15642	A	19971210
ASSTONMENT HISTORY FOR HS	DATEM	TAMATTARIE	TNI I	VAIGNTE SHEET	FORMAT	

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FOR OTHER SOURCE(S): MARPAT 131:67209

GT.

- AB Claimed are certain chelates of paramagnetic metal cations, especially Gd3+, and their use for diagnostic imaging by magnetic resonance and of radiolabeled metal chelates as scintigraphic agents. Provided are chelate complexes of paramagnetic metal cations containing polyaminocarboxylic acid-substituted cyclen chelating ligands I [m = 1 or 2; R' = H, Cl-4 alkyl or hydroxylkyl, CH2CO2H, CH2COWIL22 (Zl, Z2 = H, (hydroxylated) Cl-4 alkyl), or R' = CH(CO2H) (CH2)mCONHR; R = Ph derivs. II where a = 1 or 2; Z, Z' = bond, CH2, various amide derivs., etc., Z'' = various amide derivs.; Rl-R5 = H, Br, Cl, I, various amide derivs.], and their pharmacol. acceptable salts.
- RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation as diagnostic imaging agent)

RN 227598-28-9 CAPLUS

CN Gadolinate(1-), [[1,1',1'',1'''-[(1,4,7,10-tetraazacyclododecane-1,4,7,10-tetrayl-KN1,KN4,KN7,KN10)tetrakis[[4-(carboxy-

κΟ) -1-oxo-4,1-butanediyl]iminomethylene-4,1-phenylenecarbonylimino-4,1-phenylenecarbonylimino-4,1-phenylenecarbonyl[(2-

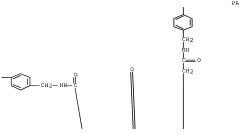
hydroxyethyl)imino]]]tetrakis[1-deoxy-D-glucitolato]](4-)]-, sodium (9CI) (CA INDEX NAME)

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PAGE 3-D

PAGE 4-B

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PAGE 5-A

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OS.CITING REF COUNT:

THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

REFERENCE COUNT:

3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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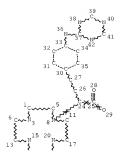
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STEREO ATTRIBUTES: NONE

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L6 2458 SEA FILE=REGISTRY SUB=L4 SSS FUL L3

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Page 1-A

Page 2-A NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

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STEREO ATTRIBUTES: NONE

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L39 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2010 ACS on STN ACCESSION NUMBER: 2004:1156521 CAPLUS Full-text

DOCUMENT NUMBER: 142:94136

TITLE: Preparation of peptidyl gadolinium contrast agents having specific high-relaxivity

INVENTOR(S): Port, Marc; Rousseaux, Olivier; Corot, Claire;

Prigent, Philippe; Lancelot, Eric

PATENT ASSIGNEE(S): Guerbet, Fr. SOURCE:

PCT Int. Appl., 179 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2 PATENT INFORMATION:

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		RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,		
			ΑZ,	BY,	KG,	KΖ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,		
			EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	ΙT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,		
			SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,		
			SN,	TD,	TG															
F	FR 2856689					A1 20041231				FR 2003-7694						20030625				
E	ΣP	1635	877			A2 20060322			0322	EP 2004-743857						20040617				
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙT,	LI,	LU,	NL,	SE,	MC,	PT,		
			ΙE,	SI,	FI,	RO,	CY,	TR,	BG,	CZ,	EE,	HU,	PL,	SK						
Ü	JS	2006	0239	926		A1	A1 20061026			US 2004-560830						20040617				
J	ΓP	2007	5278	57		T		2007	1004	JP 2006-516592						2	0040	617		
PRIORI	TY	APP:	LN.	INFO	. :						FR 2	2003-	7694			A 2	0030	625		
											US 2	2003-	5054	23P		P 2	0030	925		
											WO 2	2004-	IB21	93		W 2	0040	617		

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

The invention relates to novel compds, and pharmaceutical compns, that are useful for the diagnosis of many pathologies, in particular cardiovascular, cancer-related and inflammatory pathologies. These compds, comprise a component for targeting a pathol, region linked to a detection component which is effective in diagnostic terms. The detection component is typically an MRI contrast agent, an X-ray contrast agent, or an entity containing a radioisotope or able to be detected by ultrasound or by optical imaging. Compds. Bx-Lz-(HR Ch)y (B is a biovector, L is a linker, HR Ch is a chelate, and x, y, z are 1-8), and their salts with pharmaceutically-acceptable acids or bases, are claimed. Thus, a gadolinium-complexed 1,4,7,10-tetrazacyclododecane derivative was prepared and coupled with peptide H-Pro-Leu-Gly-NHOH. A bis-folate derivative shows very good molar relaxivity (53 mM-1.s-1 at 60 MHz).

IT 596121-94-7P 596122-03-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of peptidyl gadolinium contrast agents having specific high-relaxivity)

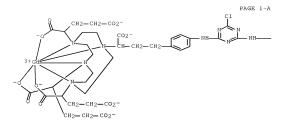
RN 596121-94-7 CAPLUS

CN Gadolinate(8-), [µ-[(a,a''''-[(6-chloro-1,3,5-triazine-2,4-diyl)bis(imino-4,1-phenylene-2,1ethanediyl)]bis(a',a'',a'''-tris(2-carboxyethyl)-

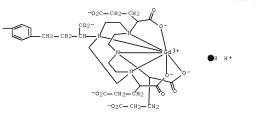
 $1,4,7,10 - {\tt tetraazacyclododecane-1},4,7,10 - {\tt tetraacetato-}$ 

KN1, KN4, KN7, KN10, KO4, KO7, KO10]](

14-)]]di-, octahydrogen (9CI) (CA INDEX NAME)



PAGE 1-B



596122-03-1 CAPLUS RN

CN Gadolinate(4-),  $[\mu-[\alpha 3,\alpha 3'-[(6-chloro-1,3,5-triazine-2,4$ diyl)bis(imino-4,1-phenylene-2,1-ethanediyl)]bis[α6,α9-bis(2carboxyethyl)-3,6,9,15-tetraazabicyclo[9.3.1]pentadeca-1(15),11,13-triene-3,6,9-triacetato-KN3,KN6,KN9,KN15,KO3,.kappa

.06, KO9]](10-)]]di-, tetrahydrogen (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD

(2 CITINGS)

REFERENCE COUNT: THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L39 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2010 ACS on STN ACCESSION NUMBER: 2003:719481 CAPLUS Full-text

DOCUMENT NUMBER: 139:254313

TITLE:

Gadolinium chelate oligomers, their use as contrast products in magnetic resonance imaging and their

synthetic intermediates

INVENTOR(S): Nachman, Isabelle; Port, Marc; Raynal, Isabelle; Rousseaux, Olivier

PATENT ASSIGNEE(S): Guerbet SA, Fr.

SOURCE: PCT Int. Appl., 122 pp.

CODEN: PIXXD2 DOCUMENT TYPE: Patent LANGUAGE: French FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	TENT :				KIND DATE								DATE					
WO	2003	0745	23		A2 20030912 A3 20040325													
	W: AE, AG, AL,			AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,		
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US	2007	0098	643		A1		2007	0503		US 2	004-	5058	20040903					
PRIORITY	Y APP	LN.	INFO	.:						FR 2	002-	2791		A 20020305				
										WO 2	003-	FR71	W 20030305					

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

- \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT \*
- AB The invention concerns macrocyclic high-relaxivity gadolinium chelate oligomers of formula W-(A)m, wherein W, A and m represent a wide variety of polynuclear gadolinium DOTA amide analogs, and their use as contrast products with vascular remanence for magnetic resonance imaging. Example compds., e.g., I, are prepared and exhibit strong relaxivity.
- IT 596121-54-9P
  - RL: DGN (Diagnostic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
    - (preparation of gadolinium chelate oligomers as contrast agents in magnetic resonance imaging)
- RN 596121-54-9 CAPLUS
- CN Gadolinate(6-), [μ3-[[α3,α3',α3''-[1,3,5-triazine-
  - 2,4,6-triyltris(imino-4,1-phenylene-2,1-ethanediyl)|tris[ $\alpha$ 6, $\alpha$ 9-bis(2-carboxyethyl)-3,6,9,15-tetraazabicyclo[9,3.1]pentadeca-1(15),11,13-triene-3,6,9-triacetato- $\kappa$ N3. $\kappa$ N6, $\kappa$ N9, $\kappa$ N15, $\kappa$ O3
  - ,κ06,κ09]](15-)][tri-, hexahvdrogen (9CI) (CA INDEX NAME)

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IT 596121-88-9P 596121-94-7P 596122-03-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

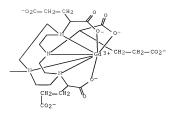
(preparation of gadolinium chelate oligomers as contrast agents in magnetic resonance imaging)

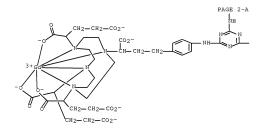
RN 596121-88-9 CAPLUS

CN Gadolinate(12-),  $[\mu 3 - [\alpha,\alpha'\cdots,\alpha'\cdots'-1,3,5-triazine-2,4,6-triy]tris(imino-4,1-phenylene-2,1-ethanediy1)]tris[a',a'',a'''-tris(2-carboxyethy1)-1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraacetato-kN1,kN4,kN7,kN10,kO4,kO7,kO10]](21-)][tri-, dodecahydrogen (9CI) (CA INDEX NAME)$ 

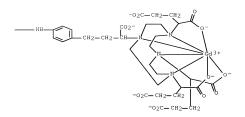
PAGE 1-A

PAGE 1-B





PAGE 2-B

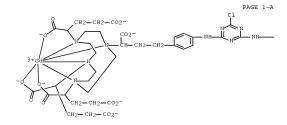


PAGE 3-A

●12 H+

RN 596121-94-7 CAPLUS

CN Gadolinate(8-), [\mu-[\(\alpha\_-\)\)[\(\alpha\_-\)\] [\(\alpha\_-\)\] [\(\alpha\_-\)\] [\(\alpha\_-\)\] [\(\alpha\_-\)\] [\(\alpha\_-\)\] (6-chloro-1,3,5-triazine-2,4-diyl) bis (\(\alpha\_+\)\) [\(\alpha\_+\)\] (2-carboxyethyl) - 1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraacetato-kNl,kNl,kNl,kNl),kNl,kO,kOl]] (14-)] [\(\alpha\_+\)] [\(\alpha\_+\)\] (3-(a) ctahydrogen (9CI) (CA INDEX NAME)



PAGE 1-B

RN 596122-03-1 CAPLUS

CN Gadolinate(4-), [μ-[(α3,α3'-[(6-chloro-1,3,5-triazine-2,4-diyl)bis(imino-4,1-phenylene-2,1-ethanediyl)]bis(α6,α9-bis(2-carboxyethyl)-3,6,9,15-tetraazabicyclo[9.3.1]pentadeca-1(15),11,13-triene-3,6,9-triacetato-κN3, κN6, κN9, κN15, κΟ3, .kappa .0.6, κ09][(10-)]ldj-, tetrahydrogen (9CI) (CA INDEX NAME)

PAGE 1-A

■4 H+

PAGE 1-B

OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD

(9 CITINGS)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his ful

L9

(FILE 'HOME' ENTERED AT 14:27:01 ON 21 JUL 2010)

FILE 'REGISTRY' ENTERED AT 14:27:06 ON 21 JUL 2010

L1 1 SEA SPE=ON ABB=ON PLU=ON PORPHYRIN/CN

FILE 'REGISTRY' ENTERED AT 14:27:42 ON 21 JUL 2010

L2 STR 101-60-0

L\*\*\* DEL 3 S L2 EXA SAM

L3 STR L2

L4 47225 SEA SPE=ON ABB=ON PLU=ON GD/ELS

L5 50 SEA SUB=L4 SSS SAM L3

L6 2458 SEA SUB=L4 SSS FUL L3

FILE 'CAPLUS' ENTERED AT 14:29:15 ON 21 JUL 2010

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D SCA

D IBIB

E US2003-505423P/APPS

L8 2 SEA SPE=ON ABB=ON PLU=ON US2003-505423P/PRN

D SCA TI

D IBIB TOT 2 SEA SPE=ON ABB=ON PLU=ON L8 AND GADOLIN?

L10 1 SEA SPE=ON ABB=ON PLU=ON L8 AND GADOLIN?/TI

SEL RN

FILE 'REGISTRY' ENTERED AT 14:34:06 ON 21 JUL 2010

L11 123 SEA SPE—ON ABB=ON PLU—ON (103145-74-0/BI OR 108-77-0/BI OR 111431-25-5/BI OR 112245-041-2/BI OR 119-24-4/BI OR 108-12143-82-6/BI OR 127903-20-2/BI OR 128184-06-5/BI OR 130707-80-1/BI OR 1499-55-4/BI OR 1947-00-8/BI OR 194920-62-2/BI OR 197151-66-9/BI OR 197151-66-9/BI OR 197151-68-1/BI OR 197151-79-4/BI OR 226559-04-2/BI OR 294-90-6/BI OR 308240-98-4/BI OR 35661-39-3/BI OR 35737-15-6/BI OR 391902-88-5/BI OR 407-25-0/BI OR

4246-51-9/BI OR 5231-87-8/BI OR 53464-60-1/BI OR 55941-86-1/BI OR 59-30-3/BI OR 596121-50-5/BI OR 596121-51-6/BI OR 596121-55-0/BI OR 596121-56-1/BI OR 596121-57-2/BI OR 596121-58-3/BI OR 596121-59-4/BI OR 596121-70-9/BI OR 596121-71-0/BI OR 596121-72 -1/BI OR 596121-73-2/BI OR 596121-75-4/BI OR 596121-76-5/BI OR 596121-77-6/BI OR 596121-78-7/BI OR 596121-90-3/BI OR 596121-92 -5/BI OR 596121-94-7/BI OR 596122-03-1/BI OR 597559-21-2/BI OR 597559-94-9/BI OR 597564-14-2/BI OR 69747-36-0/BI OR 7209-00-9/ BI OR 760-94-1/BI OR 7738-22-9/BI OR 78668-34-5/BI OR 78888-18-3/BI OR 819051-18-8/BI OR 819074-44-7/BI OR 819074-45-8/BI OR 819074-46-9/BI OR 819074-47-0/BI OR 819074-48-1/BI OR 819074-49 -2/BI OR 819074-50-5/BI OR 819074-51-6/BI OR 819074-52-7/BI OR 819074-53-8/BT OR 819074-54-9/BT OR 819074-55-0/BT OR 819074-56 -1/BI OR 819074-57-2/BI OR 819074-58-3/BI OR 819074-59-4/BI OR 819074-60-7/BI OR 819074-61-8/BI OR 819074-62-9/BI OR 819074-63 -0/BI OR 819074-64-1/BI OR 819074-65-2/BI OR 819074-66-3/BI OR 819074-67-4/BT OR 819074-68-5/BT OR 819074-69-6/BT OR 819074-70 -9/BI OR 819074-71-0/BI OR 819074-72-1/BI OR 819074-73-2/BI OR 819074-74-3/BI OR 819074-75-4/BI OR 819074-76-5/BI OR 819074-77 -6/BI OR 819074-78-7/BI OR 819074-79-8/BI OR 819074-80-1/BI OR 819074-81-2/BI OR 819074-82-3/BI OR 819074-83-4/BI OR 819074-84 -5/BI OR 819074-85-6/BI OR 819074-86-7/BI OR 819074-87-8/BI OR 81907

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L12
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L13
            10 SEA SPE=ON ABB=ON PLU=ON L12 AND L6
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FILE 'STNGUIDE' ENTERED AT 14:35:26 ON 21 JUL 2010

FILE 'REGISTRY' ENTERED AT 15:00:10 ON 21 JUL 2010

L15 STR L3

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3 SEA SPE=ON ABB=ON PLU=ON L17 AND L11 L18

D SCA

10 SEA SPE=ON ABB=ON PLU=ON L6 AND L11

L19 L20 7 SEA SPE-ON ABB-ON PLU-ON L19 NOT L18

L21 STR L15

L26

L22 22 SEA SUB=L6 SSS SAM L21 L23

570 SEA SUB=L6 SSS FUL L21

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61 SEA SPE=ON ABB=ON PLU=ON L24 AND (PY<2004 OR AY<2004 OR

PRY<2004)

FILE 'REGISTRY' ENTERED AT 15:12:15 ON 21 JUL 2010 STR L21

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L29 86 SEA SUB=L6 SSS FUL L27 L30

2 SEA SPE=ON ABB=ON PLU=ON L29 AND L11 D SCA

FILE 'CAPLUS' ENTERED AT 15:16:52 ON 21 JUL 2010 L31 20 SEA SPE=ON ABB=ON PLU=ON L29

FILE 'REGISTRY' ENTERED AT 15:17:03 ON 21 JUL 2010

L32 STR L27 L33 14 SEA SUB=L29 SSS FUL L32

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L35 2 SEA SPE=ON ABB=ON PLU=ON L25 AND L34

FILE 'REGISTRY' ENTERED AT 15:21:05 ON 21 JUL 2010

L36 STR L3

FILE 'CAPLUS' ENTERED AT 15:23:57 ON 21 JUL 2010 L39 2 SEA SPE=ON ABB=ON PLU=ON L38

FILE 'CAPLUS' ENTERED AT 15:24:13 ON 21 JUL 2010

D QUE L25 D QUE L34 L40 7 SEA SPE=ON ABB=ON PLU=ON L25 OR L

7 SEA SPE=ON ABB=ON PLU=ON L25 OR L34 D L40 IBIB ABS HITSTR TOT

D OUE L39

D L39 IBIB ABS HITSTR TOT

## FILE HOME

## FILE REGISTRY

Property values tagged with IC are from the  ${\tt ZIC/VINITI}$  data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 JUL 2010 HIGHEST RN 1233120-12-1 DICTIONARY FILE UPDATES: 19 JUL 2010 HIGHEST RN 1233120-12-1

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## FILE CAPLUS

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FILE COVERS 1907 - 21 Jul 2010 VOL 153 ISS 4

FILE LAST UPDATED: 20 Jul 2010 (20100720/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2010

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2010

CAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2010.

CAS Information Use Policies apply and are available at:

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This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Jul 16, 2010 (20100716/UP).